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Variational Solutions of the Hubbard Model for the bcc Lattice

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Abstract

A variational method is used to find approximative solutions of the Hubbard model for the ground state of the bcc lattice in the weak and strong coupling limits. The neutral case (a half-filled band) is found to be antiferromagnetic for all values of the coupling constant. However, for other choices of the band-filling second phase transitions between different magnetic structures are found if the coupling constant is varied.

1. Introduction

Numerous studies have been done of the Hubbard model (Hubbard 1963, 1964*a*, 1964*b*) for systems such as finite one-dimensional chains (Olés *et al.* 1986), four-point systems (Heinig and Monecke 1972; Heinig *et al.* 1972) and real lattices (Dichtel *et al.* 1971; Steeb and Marsch 1974; Grensing *et al.* 1978). In Wannier representation, the Hubbard Hamiltonian has the form

$$\hat{H} = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where the summations are performed over all lattice sites and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ is the number operator. Owing to numerical complexity, the majority of these studies only discuss the neutral system, i.e. $n_e \equiv N_e/N = 1$, where N is the number of lattice sites and N_e is the number of electrons.

The Hubbard model plays an important role in the modelling of magnetism, charge density waves and high-T_c superconductivity, since the interaction term of the Hubbard Hamiltonian can be written (Villet and Steeb 1990) as

$$n_{i\uparrow} n_{i\downarrow} \equiv \tfrac{1}{4}(1-\alpha_i) + \hat{R}_{iz} + \tfrac{1}{3}(\alpha_i - 1)\mathbf{S}_i^2 + \tfrac{1}{3}(\alpha_i + 1)\mathbf{R}_i^2. \tag{2}$$

Here $\mathbf{S}_i$ are the spin operators

$$\begin{aligned} \hat{S}_{ix} &= \tfrac{1}{2}(c_{i\uparrow}^{\dagger} c_{i\downarrow} + c_{i\downarrow}^{\dagger} c_{i\uparrow}), \\ \hat{S}_{iy} &= \frac{1}{2i}(c_{i\uparrow}^{\dagger} c_{i\downarrow} - c_{i\downarrow}^{\dagger} c_{i\uparrow}), \\ \hat{S}_{iz} &= \tfrac{1}{2}(n_{i\uparrow} - n_{i\downarrow}), \end{aligned} \tag{3}$$

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and $\mathbf{R}_i$ are the quasi-spin operators

$$\hat{R}_{ix} = \tfrac{1}{2}(c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} + c_{i\downarrow} c_{i\uparrow}),$$
$$\hat{R}_{iy} = \frac{1}{2i}(c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} - c_{i\uparrow} c_{i\downarrow}),$$
$$\hat{R}_{iz} = \tfrac{1}{2}(n_{i\uparrow} + n_{i\downarrow} - 1). \tag{4}$$

Both the spin operators and quasi-spin operators form a Lie algebra under the commutator.

In the present investigation a variational technique is used to investigate the ground state of the Hubbard model for the bcc lattice for various values of n_e, and the dependence of the magnetic structure on the number of electrons per lattice site n_e is found. A similar study (Penn 1966) was made for the sc lattice, but only for the weak-coupling case. Here both the weak ($t > U$) and strong ($U \gg t$) coupled regimes are considered. In the light of the above discussion it is foreseen that the the same variational technique can also be used to investigate charge ordering ($\langle R_{iz} \rangle \neq 0$) or high T_c superconductivity ($\langle R_{ix} \rangle \neq 0$).

2. The Variational Principle

Up to the present, the Hubbard Hamiltonian has been solved exactly for finite dimensional cases such as finite one-dimensional chains and a four-point system. Moreover, for the linear chain with cyclic boundary conditions, the ground state energy can be found (Lieb and Wu 1968) exactly with the help of the Bethe ansatz for $N \to \infty$, $N_e \to \infty$, $n_e = 1$ and $S_z = 0$. For more realistic systems, only approximative solutions can be found for the model. In particular, variational methods have been used widely in previous investigations. In general, two approaches are possible. In the first approach, the wave function of the system is varied to find an optimal solution for the ground state energy. The most well-known procedure of this kind is that of Gutzwiller (Gutzwiller 1963; Hashimoto 1985; Metzner and Volhardt 1987).

In the present study the second approach, in which the Hamiltonian is varied, is used to find an upper bound for the thermodynamic potential. This procedure is due to Mermin (1963). A trial Hamiltonian is varied to find an upper bound to the grand thermodynamic potential Ω. The same result as in this theorem can be obtained by specifying the grand canonical density matrix $\hat{W}$ as the statistical operator which minimises the grand thermodynamic potential

$$\Omega = \mathrm{tr}\hat{W}(\hat{H} - \mu\hat{N}_e) + \frac{1}{\beta}\mathrm{tr}\hat{W}\ln\hat{W} \tag{5}$$

for all hermitean $\hat{W}$ with unit trace. Here $\hat{N}_e$ is the number operator, μ is the chemical potential and $\beta = 1/k_B T$, with T the temperature and k_B the Boltzmann constant. Demanding $\delta\Omega = 0$, one finds the unique result

$$\hat{W} = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{tr}e^{-\beta(\hat{H}-\mu\hat{N})}}. \tag{6}$$

Since $\delta^2\Omega \geq 0$, (5) is indeed minimised by (6).

In almost all interacting systems the traces in (5) cannot be calculated for the operator in (6). An upper bound to Ω is therefore found by minimising (5) over a more restricted class of trial density matrices which are chosen by considering the behaviour of the system for limiting cases of the model.

In the present investigation, different choices are made for the strong and weak limits of the Hubbard Hamiltonian. The results are obtained for finite temperature, and are straightforwardly simplified for the ground state.

3. The Weak-coupling Limit

In Bloch representation the Hubbard Hamiltonian has the form

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{U}{N} \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} \delta(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4) c^{\dagger}_{\mathbf{k}_1\uparrow} c_{\mathbf{k}_2\uparrow} c^{\dagger}_{\mathbf{k}_3\downarrow} c_{\mathbf{k}_4\downarrow}, \tag{7}$$

where $\mathbf{k}$ runs over the first Brillouin zone and δ denotes the Kronecker symbol. The band energy is given by

$$\epsilon(\mathbf{k}) = \sum_{nm} t_{nm} e^{-i(\mathbf{R}_n - \mathbf{R}_m)},$$

where t_{nm} is the hopping integral and the $\mathbf{R}_n$ are lattice vectors.

When considering the Hubbard model in the weak-coupling limit ($U < t$, where t is the hopping integral for the nearest-neigbour terms in the expression for the band energy), inspection of (7) suggests that a useful form of the trial density matrix would be

$$W_{trial} = \frac{e^{-\beta\hat{O}}}{\mathrm{tr} e^{-\beta\hat{O}}},$$

with

$$\hat{O} = \sum_{\mathbf{k}} [E_1(\mathbf{k}) c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} + E_2(\mathbf{k}) c^{\dagger}_{\mathbf{k}\downarrow} c_{\mathbf{k}\downarrow}].$$

However, this form does not allow the incorporation of the magnetic structure of the system into the theory. This is achieved by the introduction of a unitary transformation for the operators in Bloch representation:

$$A = e^{iS} \bar{A} e^{-iS}. \tag{8}$$

Here the operator A can either be $c^{\dagger}_{\mathbf{k}\sigma}$ or $c_{\mathbf{k}\sigma}$ and S is a hermitean operator given by

$$S = \frac{i}{2} \sum_{\mathbf{k}} (\alpha_{\mathbf{k}} \bar{c}^{\dagger}_{\mathbf{k}\uparrow} \bar{c}_{\mathbf{k}+\mathbf{Q}\downarrow} - \alpha_{\mathbf{k}} \bar{c}^{\dagger}_{\mathbf{k}+\mathbf{Q}\downarrow} \bar{c}_{\mathbf{k}\uparrow}). \tag{9}$$

It follows from (8) that

$$\begin{pmatrix} \bar{c}_{\mathbf{k}\uparrow}^{(\dagger)} \\ \bar{c}_{\mathbf{k}+\mathbf{Q}\downarrow}^{(\dagger)} \end{pmatrix} = \begin{pmatrix} \cos\frac{\alpha_{\mathbf{k}}}{2} & \sin\frac{\alpha_{\mathbf{k}}}{2} \\ -\sin\frac{\alpha_{\mathbf{k}}}{2} & \cos\frac{\alpha_{\mathbf{k}}}{2} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow}^{(\dagger)} \\ c_{\mathbf{k}+\mathbf{Q}\downarrow}^{(\dagger)} \end{pmatrix}, \tag{10}$$

and the trial operator becomes

$$W_{trial} = \frac{\exp(-\beta \sum_{\mathbf{k}} [E_1(\mathbf{k}) \bar{c}_{\mathbf{k}\uparrow}^{\dagger} \bar{c}_{\mathbf{k}\uparrow} + E_2(\mathbf{k}) \bar{c}_{\mathbf{k}\downarrow}^{\dagger} \bar{c}_{\mathbf{k}\downarrow}])}{\operatorname{tr} \exp(-\beta \sum_{\mathbf{k}} [E_1(\mathbf{k}) \bar{c}_{\mathbf{k}\uparrow}^{\dagger} \bar{c}_{\mathbf{k}\uparrow} + E_2(\mathbf{k}) \bar{c}_{\mathbf{k}\downarrow}^{\dagger} \bar{c}_{\mathbf{k}\downarrow}])}. \tag{11}$$

In this approach, the quantities $E_1(\mathbf{k})$, $E_2(\mathbf{k})$, $\alpha_{\mathbf{k}}$ and $\mathbf{Q}$ are variational parameters. The physical significance of the vector $\mathbf{Q}$ is discussed in Section 6.

Using the requisite form of Wick's theorem, the traces in (5) can now be calculated and the thermodynamic potential can be written in terms of the basic quantities

$$\begin{aligned} < \bar{c}_{\mathbf{k}\uparrow}^{\dagger} \bar{c}_{\mathbf{k}\uparrow} > &= [1 + e^{\beta E_1(\mathbf{k})}]^{-1} := f_1(\mathbf{k}), \\ < \bar{c}_{\mathbf{k}\downarrow}^{\dagger} \bar{c}_{\mathbf{k}\downarrow} > &= [1 + e^{\beta E_2(\mathbf{k})}]^{-1} := f_2(\mathbf{k}), \end{aligned} \tag{12}$$

as well as the gap

$$\Delta = \frac{U}{N} \sum_{\mathbf{k}} < c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}+\mathbf{Q}\downarrow} > = \frac{U}{2N} \sum_{\mathbf{k}} \sin\alpha_{\mathbf{k}} [f_2(\mathbf{k}+\mathbf{Q}) - f_1(\mathbf{k})] \tag{13}$$

and the total spin of the system,

$$S_z = \tfrac{1}{2} \sum_{\mathbf{k}} < c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} - c_{\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\downarrow} > = \tfrac{1}{2} \sum_{\mathbf{k}} \cos\alpha_{\mathbf{k}} [f_2(\mathbf{k}) - f_1(\mathbf{k})]. \tag{14}$$

With the number of electrons per lattice site fixed by

$$n_e = \frac{1}{N} \sum_{\mathbf{k}\sigma} < c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} > = \frac{1}{N} \sum_{\mathbf{k}} [f_1(\mathbf{k}) + f_2(\mathbf{k}+\mathbf{Q})], \tag{15}$$

the variational conditions

$$\frac{\partial \Omega_t}{\partial \alpha_{\mathbf{k}}} = 0; \quad \frac{\partial \Omega_t}{\partial E_1} = \frac{\partial \Omega_t}{\partial E_2} = 0; \quad \frac{\partial \Omega_t}{\partial Q_i} = 0 \quad (i = 1,2,3) \tag{16}$$

then yield the quasi-particle spectrum

$$E_{1,2}(\mathbf{k}) = X_{\mathbf{k}} \pm E_{\mathbf{k}}\,, \tag{17}$$

where

$$E_{\mathbf{k}} := \left([\tfrac{1}{2}(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{Q}}) - \frac{U}{N} S_z]^2 + \Delta^2 \right)^{\frac{1}{2}}; \quad X_{\mathbf{k}} := \tfrac{1}{2}(\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}+\mathbf{Q}}) - \mu + \tfrac{1}{2} U n_e\,, \tag{18}$$

as well as the self-consistent equations

$$\Delta \left(2 - \frac{U}{N} \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}} \frac{\sinh(\beta E_{\mathbf{k}})}{\cosh(\beta E_{\mathbf{k}}) + \cosh(\beta X_{\mathbf{k}})} \right) = 0\,, \tag{19a}$$

$$\frac{2S_z}{N} + \frac{1}{N} \sum_{\mathbf{k}} \left(\frac{\tfrac{1}{2}(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{Q}}) - U S_z/N}{E_{\mathbf{k}}} \right) \left(\frac{\sinh(\beta E_{\mathbf{k}})}{\cosh(\beta E_{\mathbf{k}}) + \cosh(\beta X_{\mathbf{k}})} \right) = 0\,, \tag{19b}$$

$$n_e - 1 + \frac{1}{N} \sum_{\mathbf{k}} \frac{\sinh(\beta X_{\mathbf{k}})}{\cosh(\beta E_{\mathbf{k}}) + \cosh(\beta X_{\mathbf{k}})} = 0\,, \tag{19c}$$

$$\sum_{\mathbf{k}} g_i(\mathbf{k}+\mathbf{Q}) \frac{\sinh(\beta X_{\mathbf{k}}) - E_{\mathbf{k}}^{-1} [\tfrac{1}{2}(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{Q}}) - U S_z/N] \sinh(\beta E_{\mathbf{k}})}{\cosh(\beta E_{\mathbf{k}}) + \cosh(\beta X_{\mathbf{k}})} = 0;\ i = 1,2,3\,. \tag{19d}$$

In equation (19d) the definition

$$g_i(\mathbf{k}+\mathbf{Q}) := \frac{\partial \epsilon_{\mathbf{k}+\mathbf{Q}}}{\partial Q_i} \tag{20}$$

is used, where $i = 1,2,3$. The equations (20) can be solved simultaneously for Δ, S_z, μ and Q_i. The thermodynamic potential can then be rewritten in terms of these quantities:

$$\frac{\Omega_t}{N} = \frac{\Delta^2}{U} + U \left(\frac{S_z}{N} \right)^2 + \tfrac{1}{4} U n_e (2 - n_e) - \mu - \frac{1}{\beta} \sum_{\mathbf{k}} \ln 2[\cosh(\beta E_{\mathbf{k}}) + \cosh(\beta X_{\mathbf{k}})]\,. \tag{21}$$

4. The Strong-coupling Limit

In the strong-coupling limit ($U > t$), inspection of the Hubbard model in Wannier representation suggests that the following form of the trial operator would be useful:

$$W_{trial} = \frac{\exp(-\beta[\lambda_1 \sum_n \bar{c}_{n\uparrow}^\dagger \bar{c}_{n\uparrow} \bar{c}_{n\downarrow}^\dagger \bar{c}_{n\downarrow} + \lambda_2 \sum_n \bar{c}_{n\uparrow}^\dagger \bar{c}_{n\uparrow} + \lambda_3 \sum_n \bar{c}_{n\downarrow}^\dagger \bar{c}_{n\downarrow}])}{\operatorname{tr} \exp(-\beta[\lambda_1 \sum_n \bar{c}_{n\uparrow}^\dagger \bar{c}_{n\uparrow} \bar{c}_{n\downarrow}^\dagger \bar{c}_{n\downarrow} + \lambda_2 \sum_n \bar{c}_{n\uparrow}^\dagger \bar{c}_{n\uparrow} + \lambda_3 \sum_n \bar{c}_{n\downarrow}^\dagger \bar{c}_{n\downarrow}])}\,. \tag{22}$$

The operators $c_{i\sigma}^{(\dagger)}$ and $\bar{c}_{i\sigma}^{(\dagger)}$ respectively are the Fourier transforms of the operators $c_{\mathbf{k}\sigma}^{(\dagger)}$ and $\bar{c}_{\mathbf{k}\sigma}^{(\dagger)}$ in equation (10), and the quantities λ_1, λ_2 and λ_3 play the role of variational parameters.

The traces in (5) are calculated with the help of the appropriate version (Steeb 1976; Villet 1986) of Wick's theorem. The thermodynamic potential can then be written in terms of the distribution functions

$$\begin{aligned}
&<\uparrow\downarrow> :=< \bar{n}_{i\uparrow}\bar{n}_{i\downarrow} >= [1 + e^{\beta(\lambda_1+\lambda_2)} + e^{\beta(\lambda_1+\lambda_3)} + e^{\beta(\lambda_1+\lambda_2+\lambda_3)}],\\
&<\uparrow> :=< \bar{n}_{i\uparrow} >=<\uparrow\downarrow> [1 + e^{\beta\lambda_1+\lambda_3)}],\\
&<\downarrow> :=< \bar{n}_{i\downarrow} >=<\uparrow\downarrow> [1 + e^{\beta(\lambda_1+\lambda_2)}],
\end{aligned} \tag{23}$$

as well as the Fourier transforms

$$\begin{aligned}
S &= \frac{1}{N}\sum_{\mathbf{k}} \tfrac{1}{2}(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{Q}}) \cos\alpha_{\mathbf{k}},\\
C &= \tfrac{1}{4}U\left[1 - \left(\frac{1}{N}\sum_{\mathbf{k}} \sin\alpha_{\mathbf{k}}\right)^2 - \left(\frac{1}{N}\sum_{\mathbf{k}} \cos\alpha_{\mathbf{k}}\right)^2\right],\\
V &= \frac{U}{N^3}\sum_{\mathbf{k}_1}\left[\sum_{\mathbf{k}_2} \cos\left(\frac{\alpha_{\mathbf{k}_1-\mathbf{k}_2} - \alpha_{\mathbf{k}_2}}{2}\right)\right]^2.
\end{aligned} \tag{24}$$

The quantities $\alpha_{\mathbf{k}}$, λ_1, λ_2 and λ_3 which occur in (24) are variational parameters and are fixed by the conditions

$$\frac{\partial\Omega_t}{\partial\lambda_1} = \frac{\partial\Omega_t}{\partial\lambda_2} = \frac{\partial\Omega_t}{\partial\lambda_3} = 0; \quad \frac{\partial\Omega_t}{\partial\alpha_{\mathbf{k}}} = 0. \tag{25}$$

Owing to the involved form of (24), the last condition in (25) is not readily implemented in closed form. However, since it is straightforwardly established that the quantity Δ defined in (12) is of the order of U, it is natural to expand the quantities in (24) in terms of

$$\eta := \frac{t}{\Delta}. \tag{26}$$

In (26) and the subsequent discussion, only nearest-neighbour hopping is considered and t is the hopping strength. Denoting the number of closed paths consisting of n nearest-neighbour steps by

$$A_n = \frac{1}{N}\sum_{\mathbf{k}}\left(\frac{1}{t}\epsilon_{\mathbf{k}}\right)^n = \sum_{(\rho_1,\rho_2,\ldots,\rho_n)\in\{nn\}} \delta(\rho_1 + \rho_2 + \ldots + \rho_n), \tag{27}$$

where δ denotes the Kronecker symbol and $\{nn\}$ denotes the set of lattice

vectors connecting nearest neighbours, equations (24) now become

$$\begin{aligned} S &= t_1(A_2\eta - \tfrac{1}{2}A_4\eta^3 + \ldots), \\ C &= \tfrac{1}{4}U[A_2\eta^2 - \tfrac{1}{4}(3A_4 + A_2{}^2)\eta^4 + \ldots], \\ V &= U[1 - \tfrac{1}{2}A_2\eta^2 + \tfrac{1}{32}(11A_4 + 3A_2{}^2 + 2A_2)\eta^4 - \ldots]. \end{aligned} \tag{28}$$

With (28) taken to $O(\eta^4)$, the conditions (25) now yield the following set of self-consistent equations for λ_1, λ_2, λ_3 and η:

$$\lambda_1 = V, \tag{29a}$$

$$\lambda_2 = S - \mu + 2C(\langle\uparrow\rangle - \langle\downarrow\rangle) + \langle\downarrow\rangle\,(U - V), \tag{29b}$$

$$\lambda_3 = -S - \mu - 2C(\langle\uparrow\rangle - \langle\downarrow\rangle) + \langle\uparrow\rangle\,(U - V), \tag{29c}$$

$$U\left[\frac{y}{8}(11A_4 + 3A_2{}^2 + 2A_2) - \frac{x^2}{4}(3A_4 + A_2{}^2)\right]\eta^3 - \frac{3x}{2}A_4 t\eta^2 + UA_2\left(\frac{x^2}{2} - y\right)\eta + xtA_2 = 0. \tag{29d}$$

In (29) the definitions

$$x := \langle\uparrow\rangle - \langle\downarrow\rangle; \quad y := \langle\uparrow\downarrow\rangle - \langle\uparrow\rangle\langle\downarrow\rangle \tag{30}$$

have been used. The chemical potential μ in (29) is fixed by the number of electrons per lattice site:

$$n_e = \langle\uparrow\rangle + \langle\downarrow\rangle\,. \tag{29e}$$

The thermodynamical potential now becomes

$$\frac{\Omega_t}{N} = V - 2\mu - x^2C + (n_e - \langle\uparrow\rangle\langle\downarrow\rangle)(U - V) + \frac{1}{\beta}\ln\langle\uparrow\downarrow\rangle\,. \tag{31}$$

5. The bcc Lattice

The results in Sections 3 and 4 are quite general, except for the assumption of nearest-neighbour hopping in Section 4. In the present investigation, the bcc lattice is the model system. With nearest-neighbour hopping, the band energy in (18) is then given by

$$\epsilon_k = 8t\cos\left(\frac{k_1 a}{2}\right)\cos\left(\frac{k_2 a}{2}\right)\cos\left(\frac{k_3 a}{2}\right), \tag{32}$$

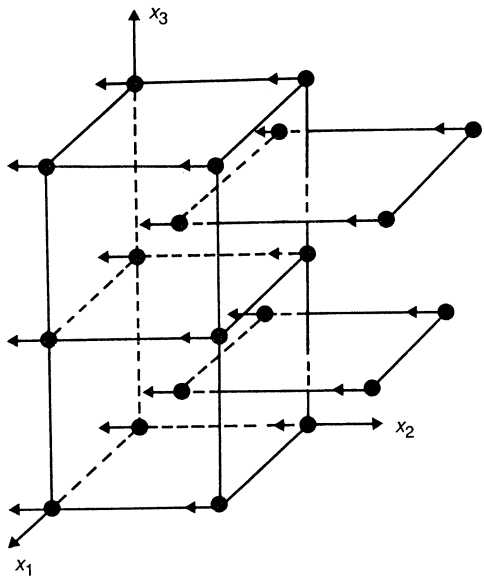

Fig. 1. Spin system for $\mathbf{Q} = 0$.

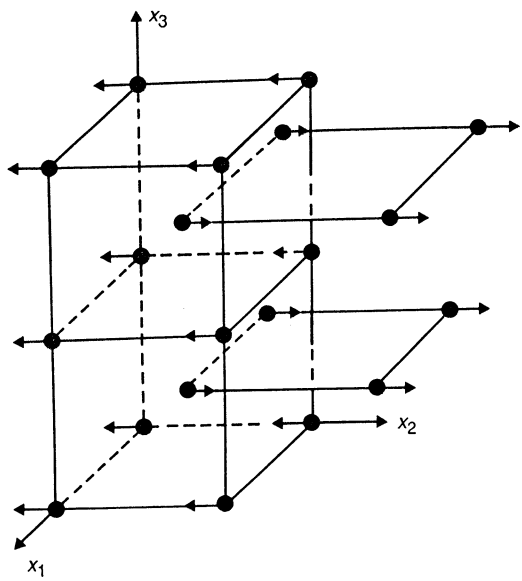

Fig. 2. Spin system for $\mathbf{Q} = 2\pi\hat{x}_3$.

where a is the cube edge. The derivative (20) becomes

$$g_i(\mathbf{k}+\mathbf{Q}) = -4at \sin\left[\frac{(k_i+Q_i)a}{2}\right]\cos\left[\frac{(k_j+Q_j)a}{2}\right]\cos\left[\frac{(k_l+Q_l)a}{2}\right] \tag{33}$$

for any permutation (ijl) of (123). In the strong coupling limit, equation (27) yields the values $A_2 = 8$; $A_4 = 216$ for the bcc lattice.

6. Magnetic Structure of System

The Coulomb interaction can be approximated by a one-particle term by the introduction of magnetic fields $\mathbf{H}_n$ at each lattice site $\mathbf{R}_n$. The contribution of these fields to the energy of the system is given by

$$H = \sum_n \tilde{c}_n^\dagger (\mathbf{H}_n.\sigma)\tilde{c}_n = \sum_n \tilde{c}_n^\dagger \begin{pmatrix} H_{nz} & H_{nx} - \mathrm{i}H_{ny} \\ H_{nx} + \mathrm{i}H_{ny} & -H_{nz} \end{pmatrix} \tilde{c}_n^T . \tag{34}$$

In (34) the components of σ are the Pauli matrices, $\tilde{c}_n^{(\dagger)}$ is the row vector $[c_{n\uparrow}^{(\dagger)}, c_{n\downarrow}^{(\dagger)}]$ and T indicates the transpose of the vector. Using the Fourier transform to Bloch representation it is then found that the rotation (9) diagonalises the Hamiltonian and that in the absence of an external field

$$H_{nx} = 2\Delta \sin(\mathbf{Q}.\mathbf{R}_n); \quad H_{ny} = -2\Delta \cos(\mathbf{Q}.\mathbf{R}_n). \tag{35}$$

The quantity $\mathbf{Q}$ can therefore be identified with a specific spin structure. Two such systems are shown for the bcc lattice in Fig. 1 (ferromagnetic case) and Fig. 2 (antiferromagnetic case).

7. Ground-state Calculations

The self-consistent equations for the weak- as well as strong-coupling limit were solved for the ground-state. The distribution functions in (12) and (23) then become step-functions, leading to some numerical difficulties for the weak-coupling limit but considerably simplifying the strong-coupling case.

From equation (19a) it is evident that in that the weak-coupling limit the solution $\Delta = 0$ always exists. This is easily identified as the paramagnetic phase of the system. This case was investigated for all values of n_e.

Numerically it was found that local minima in the ground-state energy occur for integral and half-integral values of the components of $\mathbf{Q}/\pi$. The self-consistent equations were therefore solved for all the distinguishable values to obtain the solution with lowest energy.

Since the bcc lattice is an AB lattice, the chemical potential for a half-filled band becomes $\mu = \frac{1}{2}U$, and the equations (19) and (29) are considerably simplified and reduced in number. In Fig. 3, the ground-state energy is plotted as a function of the coupling constant U for various limiting cases. Only the results for $\mathbf{Q} = 0$ (ferromagnetic phase) and $\mathbf{Q} = 2\pi\hat{z}$ (antiferromagnetic

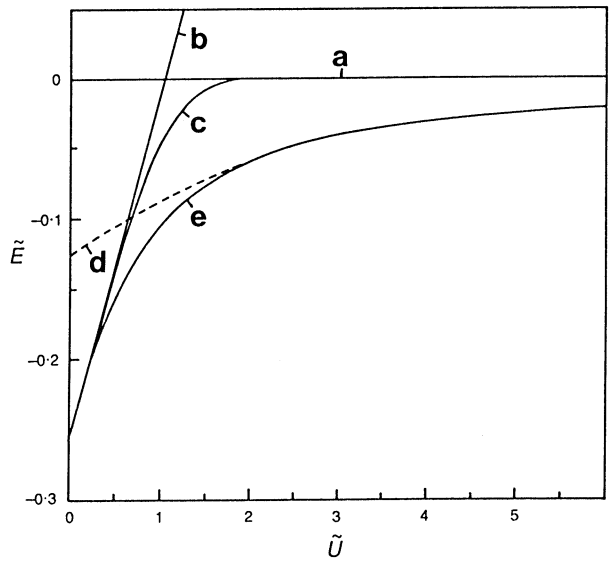

Fig. 3. The dimensionless ground-state energy $\tilde{E} = E/(8tN)$ as a function of the dimensionless coupling constant $\tilde{U} = U/(8t)$ for (a) $t = 0$, (b) the paramagnetic phase, (c) the ferromagnetic phase, (d) the antiferromagnetic phase (strong coupling) and (e) the antiferromagnetic phase (weak coupling) in the half-filled case.

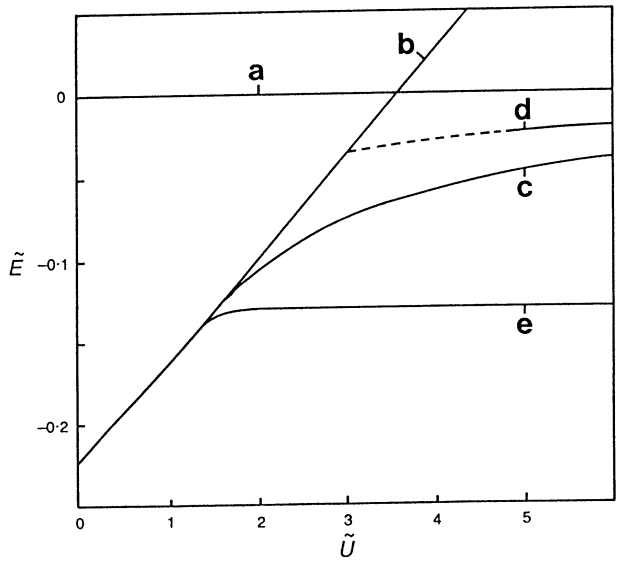

Fig. 4. The dimensionless ground-state energy $\tilde{E} = E/(8tN)$ as a function of the dimensionless coupling constant $\tilde{U} = U/(8t)$ for (a) $t = 0$, (b) the paramagnetic phase, (c) the antiferromagnetic phase (weak coupling), (d) the antiferromagnetic phase (strong coupling) and (e) the ferromagnetic phase in the quarter-filled case.

phase) are shown, since none of the other values of $\mathbf{Q}$ yield a minimum in any of the cases under consideration. It is evident from Fig. 3 that the antiferromagnetic state yields the lowest energy for all values of the coupling constant. This is in agreement with results obtained in other studies of AB lattices (Steeb and Marsch 1976; Grensing and Steeb 1978; Vanderzande 1985).

For the non-neutral case ($n_e \neq 1$), the equations (30) and (29) are solved only with some difficulty, and this case is therefore not common in the literature. In the present study, these equations were solved for a quarter ($n_e = \frac{1}{2}$) and three-quarter ($n_e = \frac{3}{2}$) filled band. Since the results are linked by particle-hole symmetry, only the quarter-filled case is discussed.

From Fig. 4 it can be seen that the ferromagnetic phase is the lowest energy solution for $U \geq 1 \cdot 5$. For lower values of U the phase seems undetermined. However, this question can be resolved by calculating the total spin of the system. From Fig. 5 it is then clear that a second-order phase transition occurs from the ferromagnetic phase to the paramagnetic phase at $U \simeq 11 \cdot 2t$. This result completely contradicts studies of finite-dimensional systems, where the ground state invariably is antiferromagnetic. It also contradicts the the results of Morris and Cornwell (1968), who find that for the sc lattice (idealised to simplify computation) the SDW state is the one of least energy. However, in a comparable study of the sc lattice (Penn 1966) the possibility of a ferromagnetic state does exist, at least for the weak-coupling domain. Though comparison with the latter author is difficult because of the different approach to the present study, as well as the fact that Penn's calculations were essentially in the weak-coupling domain, further support for a ferromagnetic state is found in the results of a rigorous study (Nagaoka 1966) of the strong-coupling behaviour of an almost half-filled band. In an investigation by Hashimoto (1985) where the Gutzwiller (1963) method was employed, ferromagnetism was also found in the bcc lattice. The phase transition in this study is found outside the ferromagnetic domain calculated by Hashimoto (1985). This discrepancy could be due to the fact that Hashimoto used an improved Gutzwiller method in the strong-coupling domain while the results of this study are essentially those of the weak-coupling limit, as is borne out by the following.

A remark is necessary on the strong-coupling limit. The truncation of the expansions in (28) leads to the result that (29d) cannot be solved for small U. Instead of entering on a laborious calculation of $O(\eta^6)$ in (28), the curve obtained from the third-order equation was extrapolated backward numerically and the extrapolated part is indicated by a dotted line in Figs 3 and 4. It is furthermore established numerically that the weak-coupling calculations consistently yield a lower ground-state energy than the strong-coupling calculations, at least for $U \leq 30t$. It therefore seems reasonable only to consider the weak-coupling limit in subsequent calculations.

From the foregoing the fact emerges that the magnetic configuration of the system in its ground state can be controlled by varying the band-filling. This is illustrated in Fig. 6, where the ground-state energy for the ferro- and antiferromagnetic phases is plotted as a function of the band-filling for a chosen value of U. It is obvious that a phase transition occurs between the two phases at $n_e \simeq 0.95$.

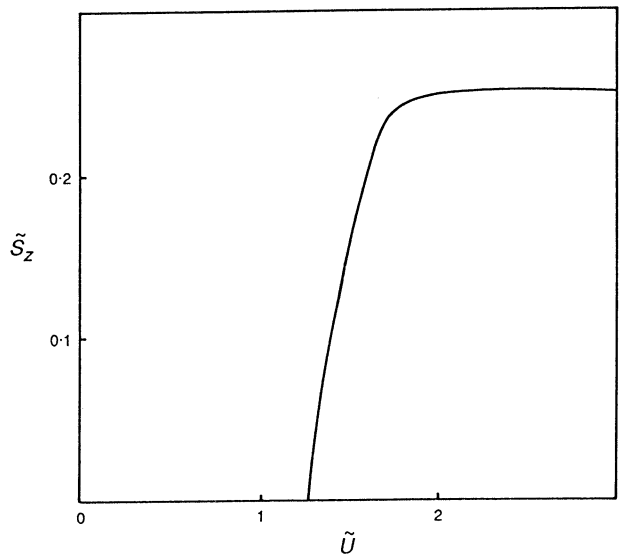

Fig. 5. The spin per lattice site $\tilde{S}_z = S_z/N$ as a function of the dimensionless coupling constant $\tilde{U} = U/(8t)$ for $n_e = \frac{1}{2}$.

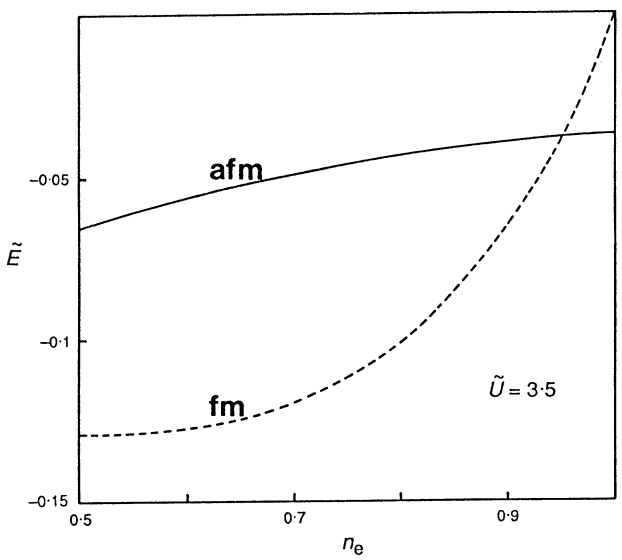

Fig. 6. The ground-state energy $\tilde{E} = E/(8t)$ as a function of the bandfilling for the ferro- (fm) and antiferromagnetic (afm) phases.

8. Summary and Conclusions

Since the Hubbard Hamiltonian is especially designed for electrons moving in a single narrow band, the theory in the present investigation will have difficulty in for instance treating the degenerate d-bands of a physical system like Cr. This limitation will be overcome in future studies by extending the model to a doubly-degenerate one, an approach that has already been used for the neutral case. Also, only nearest-neighbour hopping has been included. The limitations of this approach will be investigated in further studies by also including second nearest-neighbour hopping, an approach that also has been followed for a half-filled band in various systems. Phonon contributions to the ground state have also been ignored. An attempt to include these in the study of a finite system has already been made by Steeb *et al.* (1986).

In spite of the limitations mentioned above, the central result of this study, namely that the magnetic structure of the ground state of a system can be varied by varying the band-filling, does offer many possibilities for further studies. In particular, systems like Cr alloys, in which the magnetic behaviour can be dramatically varied by varying the number of electrons per site (Alberts and Burger 1978; Alberts and Lourens 1984), seem amenable to this approach. It is proposed that future studies be undertaken in which a properly extended Hubbard Hamiltonian will be used to investigate the behaviour of these systems in the ground state as well as at finite temperature.

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